Numerical simulation of CO_2 storage in geological formations based on a coupled Thermal-Hydraulic-Chemical model

Reactive two-phase flows in porous media appear in diverse energetic and environmental problematics. One can mention non-exhaustively geological gas storage (carbon dioxide, hydrogen or natural gases), nuclear waste management, petroleum engineering or geothermal energy production. In this talk, we will mainly focus on the application of CO_2 storage that appears as a promising way to reduce greenhouse gas emissions.

Nonisothermal reactive two-phase flows are modeled by mass conservation laws written for each chemical component in each phase (liquid or gaseous) and an energy balance equation. These equations are coupled with Darcy's law to characterize the flow velocity of each phase. Chemical reactions are described thanks to reaction rates that are either function of concentration in case of kinetic reactions or unknown for equilibrium reactions. Reaction rates at equilibrium can be eliminated by means of a linear transformation by using Morel's formalism. The chemical system is then closed with the help of mass action laws which are algebraic equations linking activities (or molar fractions) of the different species. Finally, the full system is closed by the capillary pressure law, equations of state and solubility laws characterizing each phase equilibrium. Thus, the unknowns of the system are pressures, saturations, molar fractions and the temperature. By consequence, the problem is modeled by a nonlinear system of degenerate partial differential equations (modeling the flow), coupled with algebraic or ordinary differential equations (provided by chemical reactions).

In this talk, we consider finite volume schemes for modeling nonisothermal two-phase flow coupled with geochemical interactions. Spatial discretization is carried out using a cell-centered finite volume scheme while the time discretization is performed by a Backward Differentiation Formula 2 (BDF2). The approach combines advantages of the TPFA (Two Point Flux Approximation) method to accurately solve fluxes and diffusive terms and upstream for advective terms. The nonlinear system is solved by a Newton method and a BiConjugate Gradient STABilized (BiCGSTAB) method with an AMG preconditioner is used to solve the linear systems. We aim at comparing two numerical strategies: a fully coupled fully implicit and a sequential scheme. In the fully implicit scheme, the nonlinear system gathering all equations above mentioned is solved at each time step. For the sequential solution approaches, a nonisothermal two-phase flow and a reactive transport problem are solved sequentially. These two THC modules have been implemented in the parallel open source platform DuMu^x using High Performance Computing. Numerical results for CO_2 storage in a large-scale 3D heterogeneous reservoir will be presented to demonstrate the effectiveness and efficiency of these schemes.